SuperLU: Sparse Direct Solver

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Outline

- Overview of the software
- Some background of the algorithms
  - Highlight the differences between sequential and parallel solvers
- Sparse matrix distribution and user interface
- Example program, Fortran 90 interface
- Dissection of two applications
  - Quantum mechanics (linear system)
    [M. Baertschy, C. W. McCurdy, T. N. Rescigno, W. A. Isaacs, Li]
  - Accelerator design (eigenvalue problem)
    [P. Husbands, C. Yang, Li]

What is SuperLU

- Solve general sparse linear system A x = b.
  - Example: A of dimension 10^5, only 10 ~ 100 nonzeros per row
- Algorithm: Gaussian elimination (LU factorization: A = LU), followed by lower/upper triangular solutions.
  - Store only nonzeros and perform operations only on nonzeros.
- Efficient and portable implementation for high-performance architectures; flexible interface.

Software Status

	SuperLU	SuperLU_MT	SuperLU_DIST
Platform	Serial	SMP	Distributed
Language	C	C + Pthread (or pragmas)	C + MPI
Data type	Real/complex, Single/double	Real, double	Real/complex, Double

- Friendly interface for Fortran users
- SuperLU_MT similar to SuperLU both numerically and in usage

Adoptions of SuperLU

- Industrial
  - Mathematica
  - FEMLAB
  - Python
  - HP Mathematical Library
  - NAG
- Academic/Lab:
  - In other ACTS Tools: PETSc, Hyper
  - NIMROD (simulate fusion reactor plasmas)
  - Omega3P (accelerator design, SLAC)
  - OpenSees (earthquake simluation, UCB)
  - DSpice (parallel circuit simulation, SNL)
  - Trilinos (object-oriented framework encompassing various solvers, SNL)
  - NIKE (finite element code for structural mechanics, LLNL)

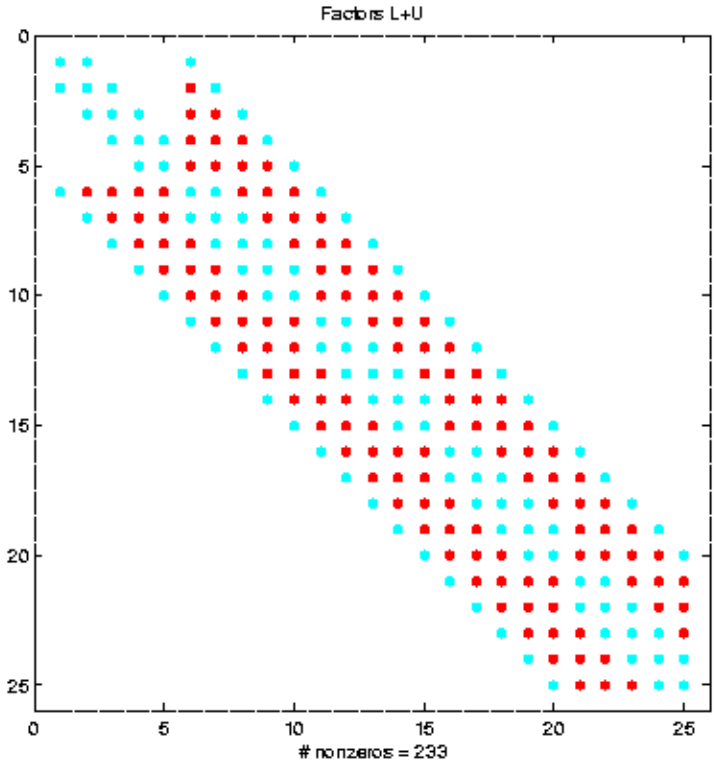
Content of SuperLU Library

- LAPACK-style interface
  - Simple and expert driver routines
  - Computational routines
  - Comprehensive testing routines and example programs
- Functionalities
  - Minimum degree ordering [MMD, Liu `85] applied to A^TA or A^T+A
  - User-controllable pivoting
    - Pre-assigned row and/or column permutations
    - Partial pivoting with threshold
  - Solving transposed system
  - Equilibration
  - Condition number estimation
  - Iterative refinement
  - Componentwise error bounds [Skeel `79, Arioli/Demmel/Duff `89]

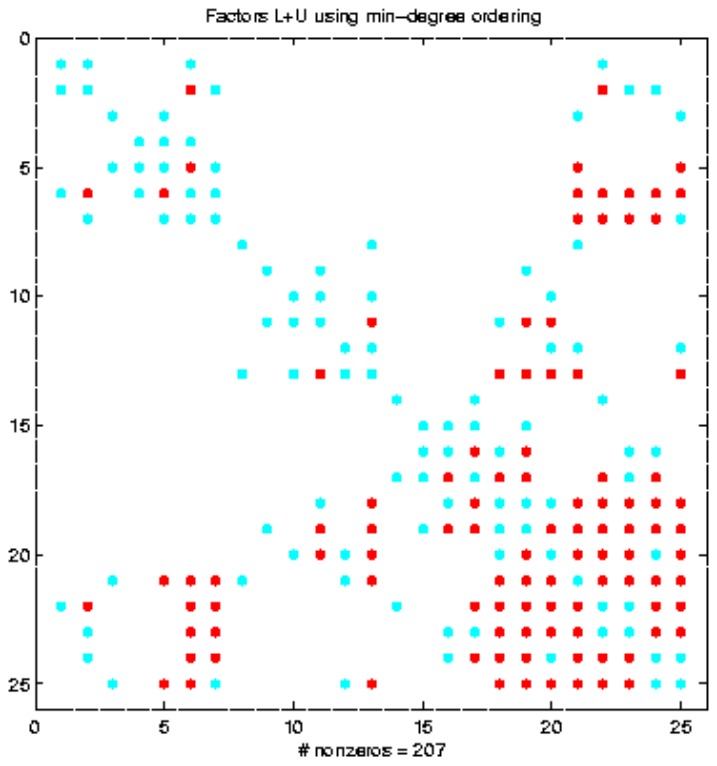
Fill-in in Sparse GE

- Original zero entry A_{ij} becomes nonzero in L or U.

Natural order: nonzeros = 233

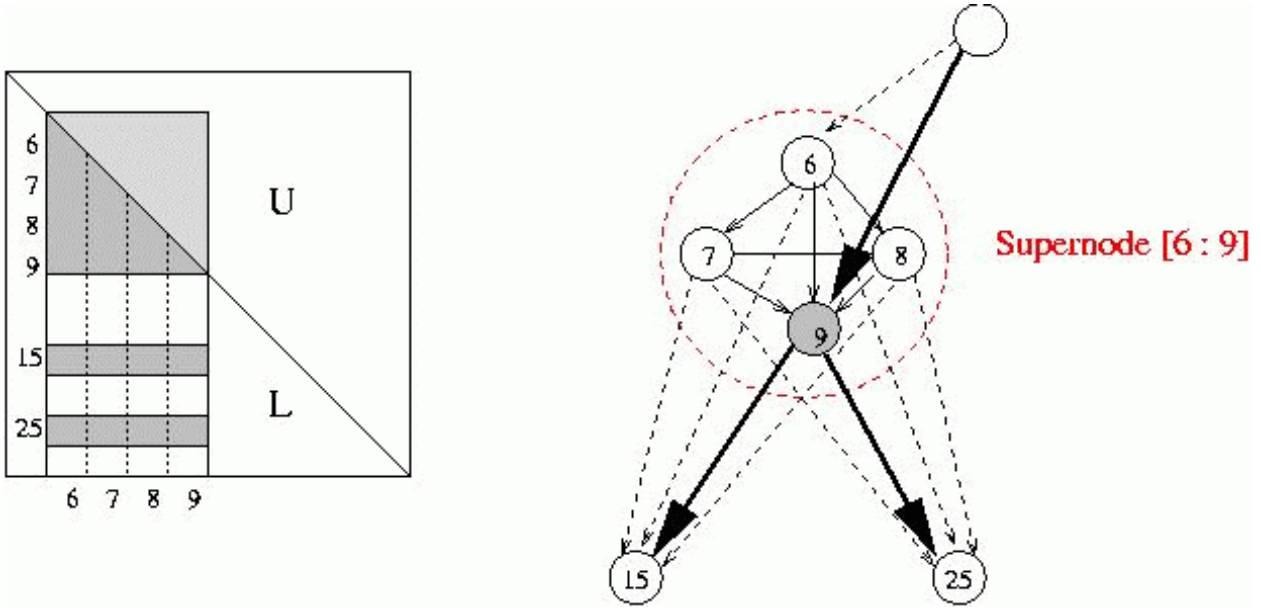


Min. Degree order: nonzeros = 207



Supernode

- Exploit dense submatrices in the L & U factors



- Why are they good?
  - Permit use of Level 3 BLAS
  - Reduce inefficient indirect addressing (scatter/gather)
  - Reduce graph algorithms time by traversing a coarser graph

Overview of the Algorithms

- Sparse LU factorization: $P_r A P_c^T = L U$
  - Choose permutations P_r and P_c for numerical stability, minimizing fill-in, and maximizing parallelism.

- Phases for sparse direct solvers
  1. Order equations & variables to minimize fill-in.
     - NP-hard, so use heuristics based on combinatorics.
  2. Symbolic factorization.
     - Identify supernodes, set up data structures and allocate memory for L & U.
  3. Numerical factorization – usually dominates total time.
     - How to pivot?
  4. Triangular solutions – usually less than 5% total time.

- Parallelization of Steps 1 and 2 are in progress.

Numerical Pivoting

- Goal of pivoting is to control element growth in L & U for stability
  - For sparse factorizations, often relax the pivoting rule to trade with better sparsity and parallelism (e.g., threshold pivoting, static pivoting , . . .)

- Partial pivoting used in sequential SuperLU (GEPP)
  - Can force diagonal pivoting (controlled by diagonal threshold)
  - Hard to implement scalably for sparse factorization

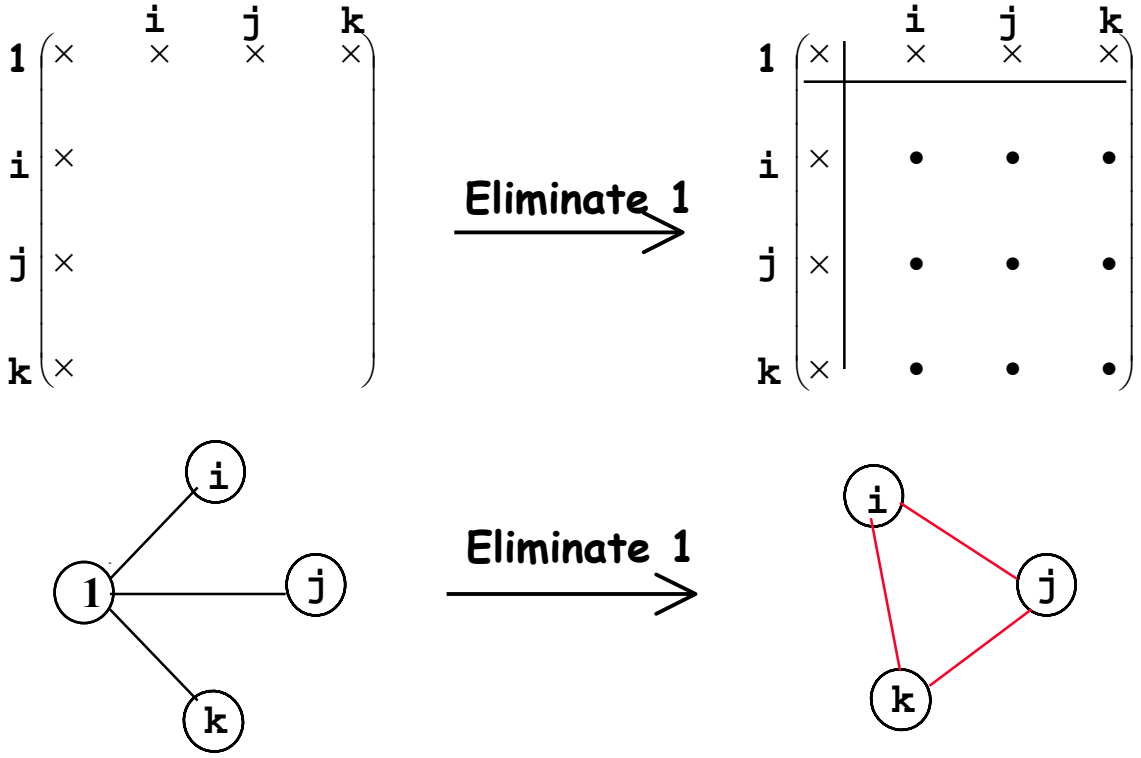
- Static pivoting used in SuperLU_DIST (GESP)
  - Before factor, scale and permute A to maximize diagonal: $P_r D_r A D_c = A'$
  - During factor $A' = LU$, replace tiny pivots by $\sqrt{\varepsilon}\|A\|$, without changing data structures for L & U
  - If needed, use a few steps of iterative refinement after the first solution

  ➔ Quite stable in practice

Ordering for Sparse Cholesky (symmetric)

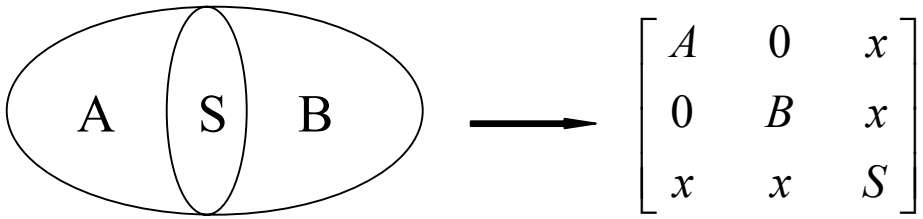
- Local greedy: Minimum degree (upper bound on fill-in)

  [Tinney/Walker `67, George/Liu `79, Liu `85, Amestoy/Davis/Duff `94, Ashcraft `95, Duff/Reid `95, et al.]



Ordering for Sparse Cholesky (symmetric)

- Global graph partitioning approach: top-down, divide-and-conqure
- Nested dissection [George '73, Lipton/Rose/Tarjan '79]
  - First level

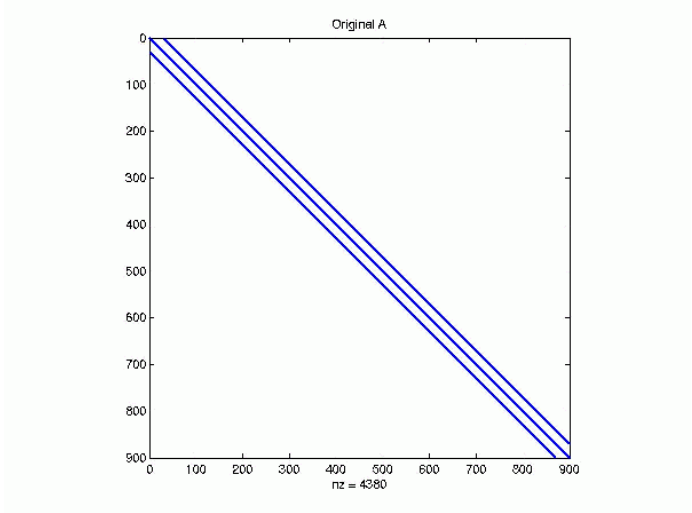


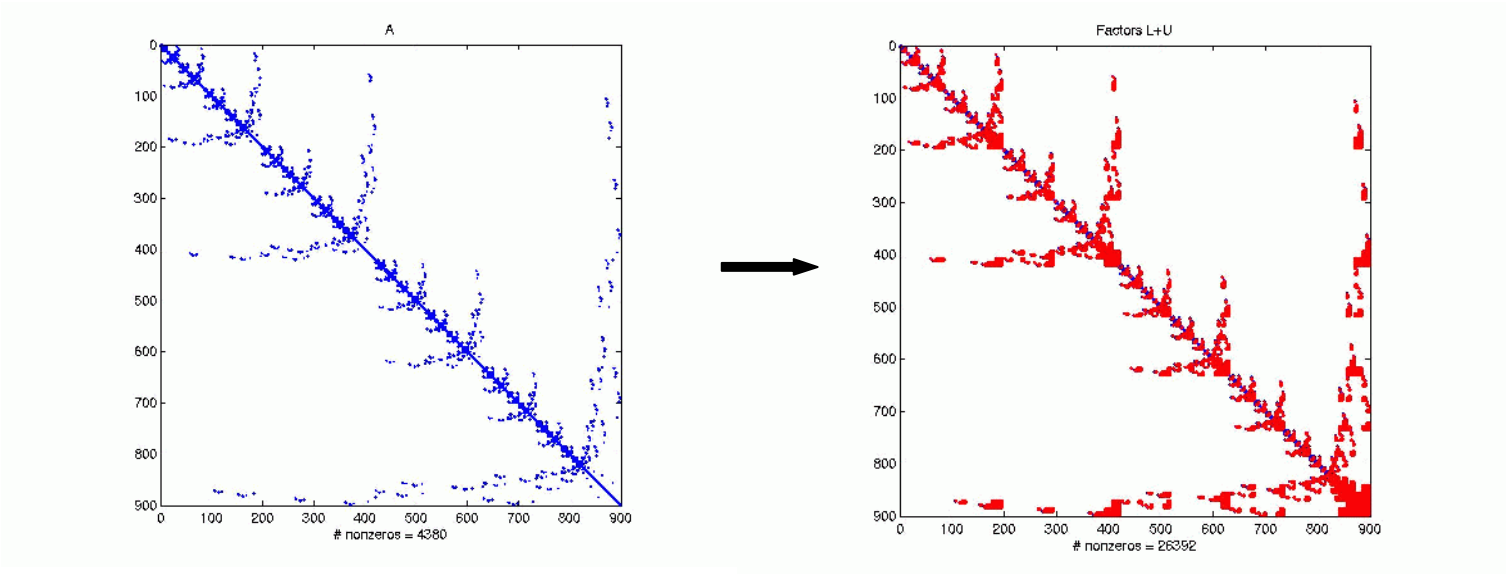
$$\begin{bmatrix} A & 0 & x \\ 0 & B & x \\ x & x & S \end{bmatrix}$$

  - Recurse on A and B

- Goal: find the smallest possible separator S at each level
  - Multilevel schemes [Hendrickson/Leland `94, Karypis/Kumar `95]
  - Spectral bisection [Simon et al. `90-`95]
  - Geometric and spectral bisection [Chan/Gilbert/Teng `94]

Ordering Based on Graph Partitioning





Ordering for LU (unsymmetric)

- Can use a symmetric ordering on a symmetrized matrix . . .
- Case of partial pivoting (sequential SuperLU):

  Use ordering based on A^TA
  - If $R^TR = A^TA$ and $PA = LU$, then for any row permutation P, struct(L+U) $\subseteq$ struct(R^T+R) [George/Ng `87]
  - Making R sparse tends to make L & U sparse . . .

- Case of static pivoting (SuperLU_DIST):

  Use ordering based on A^T+A
  - If $R^TR = A^T+A$ and $A = LU$, then struct(L+U) $\subseteq$ struct(R^T+R)
  - Making R sparse tends to make L & U sparse . . .

  - Can find better ordering based solely on A, without symmetrization [Amestoy/Li/Ng `03]

Ordering Interface in SuperLU

- Library contains the following routines:
  - Ordering algorithms: MMD [J. Liu], COLAMD [T. Davis]
  - Utilities: form A^T+A , A^TA

- Users may input any other permutation vector (e.g., using Metis, Chaco, etc.)

```
. . .
set_default_options_dist ( &options );
options.ColPerm = MY_PERMC;    /* modify default option */
ScalePermstructInit ( m, n, &ScalePermstruct );
METIS (  . . . , &ScalePermstruct.perm_c );
. . .
pdgssvx ( &options, . . . , &ScalePermstruct, . . . );
. . .
```

Ordering Comparison

		GEPP, COLAMD (SuperLU)		GESP, AMD(A^T+A) (SuperLU_DIST)	
Matrix	N	Fill (10^6)	Flops (10^9)	Fill (10^6)	Flops (10^9)
BBMAT	38744	49.8	44.6	40.2	34.0
ECL32	51993	73.5	120.4	42.7	68.4
MEMPLUS	17758	4.4	5.5	0.15	0.002
TWOTONE	120750	22.6	8.8	11.9	8.0
WANG4	26068	27.7	35.3	10.7	9.1

Symbolic Factorization

- Cholesky [George/Liu `81 book]
  - Use elimination graph of L and its transitive reduction (elimination tree)
  - Complexity linear in output: O(nnz(L))
- LU
  - Use elimination graphs of L & U and their transitive reductions (elimination DAGs) [Tarjan/Rose `78, Gilbert/Liu `93, Gilbert `94]
  - Improved by symmetric structure pruning [Eisenstat/Liu `92]
  - Improved by supernodes
  - Complexity greater than nnz(L+U), but much smaller than flops(LU)

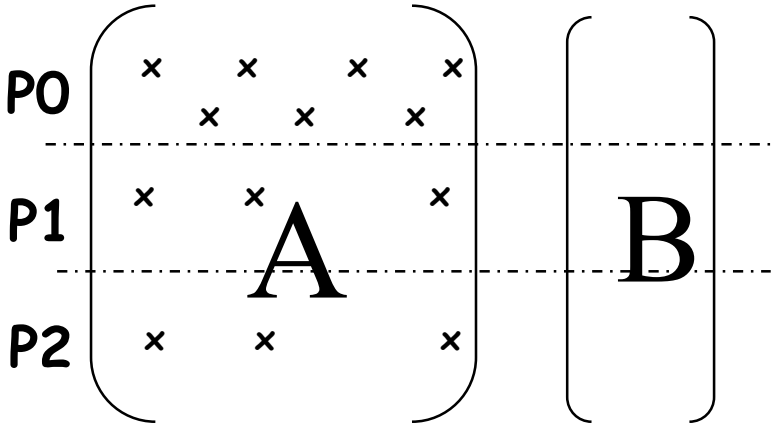
Numerical Factorization

- Sequential SuperLU
  - Enhance data reuse in memory hierarchy by calling Level 3 BLAS on the supernodes
- SuperLU_MT
  - Exploit both coarse and fine grain parallelism
  - Employ dynamic scheduling to minimize parallel runtime
- SuperLU_DIST
  - Enhance scalability by static pivoting and 2D matrix distribution

How to distribute the matrices?

- Matrices involved:
  - A, B (turned into X) – input, users manipulate them
  - L, U – output, users do not need to see them

- A (sparse) and B (dense) are distributed by block rows



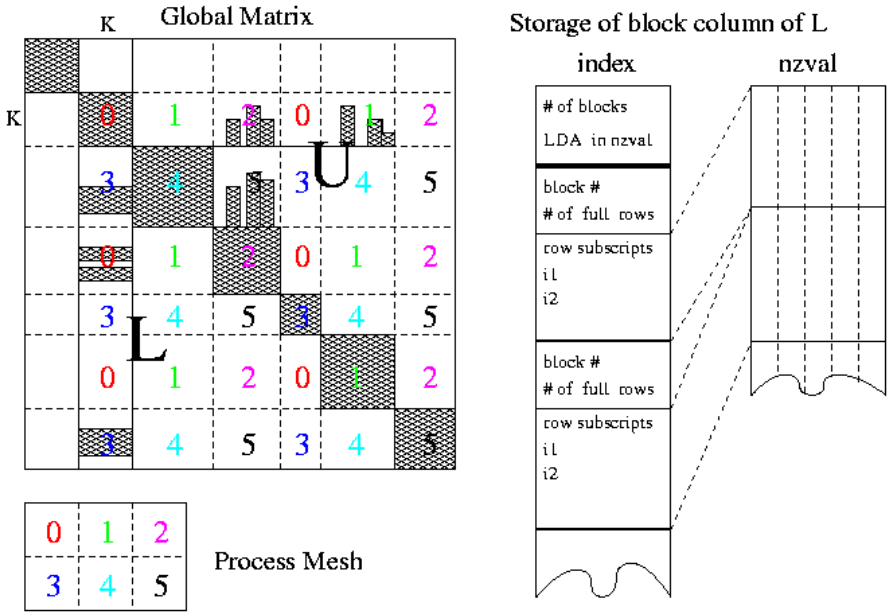
Local A stored in
Compressed Row Format

  - Natural for users, and consistent with other popular packages: PETSc, Aztec, etc.

- Each process has a structure to store local part of A (Distributed Compressed Row Format):

```
typedef struct {
    int_t   nnz_loc;  /* number of nonzeros in the local submatrix */
    int_t   m_loc;    /* number of rows local to this processor */
    int_t   fst_row;  /* global index of the first row */
    void    *nzval;   /* pointer to array of nonzero values, packed by row */
    int_t   *colind;  /* pointer to array of column indices of the nonzeros */
    int_t   *rowptr;  /* pointer to array of beginning of rows in nzval[]and colind[]  */
} NRformat_loc;
```

2D Block Cyclic Layout for L and U



- Better for GE scalability, load balance
- Library has a "re-distribution" phase to distribute the initial values of A to the 2D block-cyclic data structure of L & U.
  - All-to-all communication, entirely parallel
  - < 10% of total time for most matrices

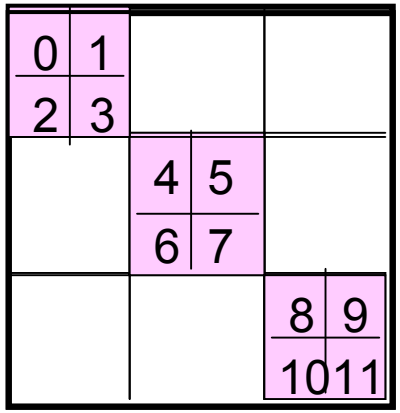
Process grid and MPI communicator

- Example: Solving a preconditioned linear system

  $M^{-1}A\ x = M^{-1}\ b$

  $M = \mathrm{diag}(A_{11}, A_{22}, A_{33})$

  → use SuperLU_DIST for each diag. block



- Need create 3 process grids, same logical ranks (0:3), but different physical ranks
- Each grid has its own MPI communicator

Two ways to create a process grid

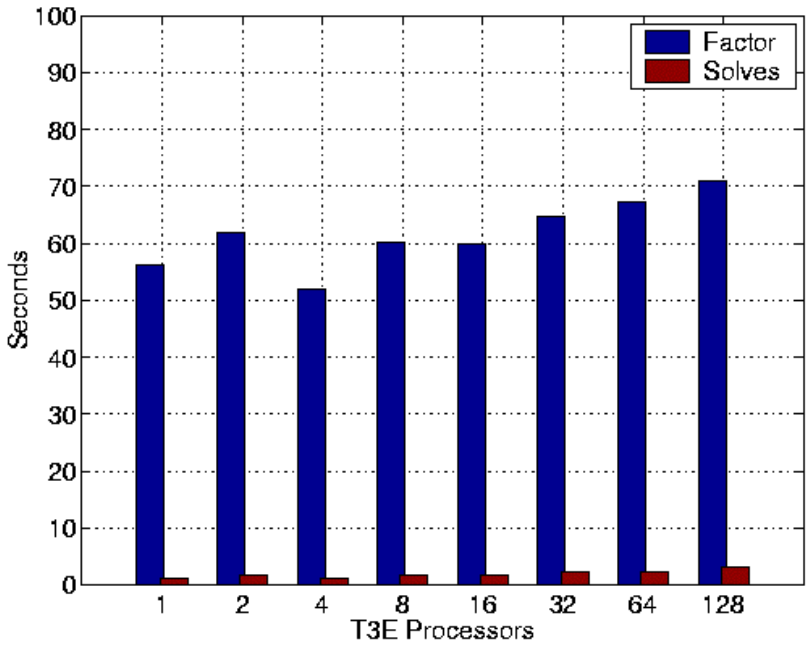
- Superlu_gridinit(MPI_Comm Bcomm, int nprow, int npcol, gridinfo_t *grid);
  - Maps the first nprow*npcol processes in the MPI communicator Bcomm to SuperLU 2D grid

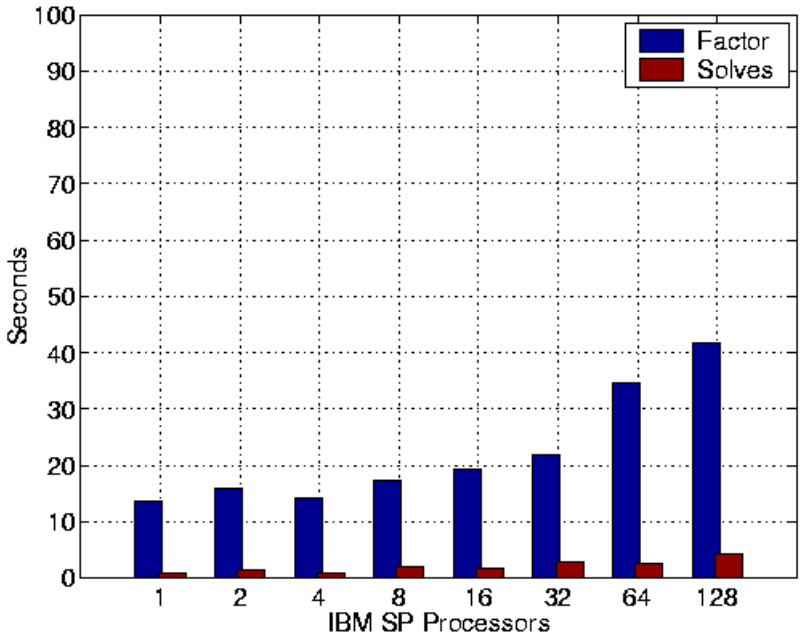
- Superlu_gridmap(MPI_Comm Bcomm, int nprow, int npcol, int usermap[], int ldumap, gridinfo_t *grid);
  - Maps an ***arbitrary*** set of nprow*npcol processes in the MPI communicator Bcomm to SuperLU 2D grid. The ranks of the selected MPI processes are given in usermap[] array. For example:

	0	1	2
0	11	12	13
1	14	15	16

Scalability

- 3D KxKxK cubic grids, scale $N^2 = K^6$ with P for constant work per processor
- Achieved 12.5 and 21.2 Gflops on 128 processors
- Performance sensitive to communication latency
  - Cray T3E latency: 3 microseconds (~ 2702 flops)
  - IBM SP latency: 8 microseconds (~ 11940 flops)





Tips for Debugging Performance

- Check ordering
- Diagonal pivoting is preferable
  - E.g., matrix is diagonally dominant, or SPD, . . .
- Need good BLAS library (vendor BLAS, ATLAS)
  - May need adjust block size for each architecture
    (Parameters modifiable in routine sp_ienv())
    - Larger blocks better for uniprocessor
    - Smaller blocks better for parallellism and load balance
  - Open problem: automatic tuning for block size?

SuperLU_DIST Example Program

- SuperLU_DIST_2.0/EXAMPLE/pddrive.c

- Five basic steps
  1. Initialize the MPI environment and SuperLU process grid
  2. Set up the input matrices A and B
  3. Set the options argument (can modify the default)
  4. Call SuperLU routine PDGSSVX
  5. Release the process grid, deallocate memory, and terminate the MPI environment

Pddrive.c

```
#include "superlu_ddefs.h“

main(int argc, char *argv[])
{
   superlu_options_t options;
   SuperLUStat_t stat;
   SuperMatrix A;
   ScalePermstruct_t ScalePermstruct;
   LUstruct_t LUstruct;
   SOLVEstruct_t SOLVEstruct;
   gridinfo_t grid;
    . . . . . .
 /* Initialize MPI environment */
   MPI_Init( &argc, &argv );
    . . . . . .
 /* Initialize the SuperLU process grid */
    nprow = npcol = 2;
    superlu_gridinit(MPI_COMM_WORLD, nprow,
                     npcol, &grid);
```

```
/* Read matrix A from file, distribute it, and set up the
   right-hand side  */
  dcreate_matrix(&A, nrhs, &b, &ldb, &xtrue, &ldx,
                       fp, &grid);


/* Set the options for the solver.  Defaults are:
      options.Fact = DOFACT;
      options.Equil = YES;
      options.ColPerm = MMD_AT_PLUS_A;
      options.RowPerm = LargeDiag;
      options.ReplaceTinyPivot = YES;
      options.Trans = NOTRANS;
      options.IterRefine = DOUBLE;
      options.SolveInitialized = NO;
      options.RefineInitialized = NO;
      options.PrintStat = YES;
   */
  set_default_options_dist(&options);
```

Pddrive.c (cont.)

```
/* Initialize ScalePermstruct and LUstruct. */
   ScalePermstructInit (m, n, &ScalePermstruct);
   LUstructInit (m, n, &LUstruct);

   /* Initialize the statistics variables. */
   PStatInit(&stat);

   /* Call the linear equation solver. */
   pdgssvx (&options, &A, &ScalePermstruct, b,
                ldb, nrhs, &grid, &LUstruct,
               &SOLVEstruct, berr, &stat, &info );

   /* Print the statistics. */
   PStatPrint (&options, &stat, &grid);

   /* Deallocate storage */
   PStatFree (&stat);
   Destroy_LU (n, &grid, &LUstruct);
   LUstructFree (&LUstruct);

   /* Release the SuperLU process grid */
   superlu_gridexit (&grid);

   /* Terminate the MPI execution environment */
   MPI_Finalize ();

}
```

Fortran 90 Interface

- SuperLU_DIST_2.0/FORTRAN/
- All SuperLU objects (e.g., LU structure) are opaque for F90
  - They are allocated, deallocated and operated in the C side and not directly accessible from Fortran side.
- C objects are accessed via handles that exist in Fortran's user space
- In Fortran, all handles are of type INTEGER

- Example:

$$A = \begin{bmatrix} s & & u & u & \\ l & u & & & \\ & l & p & & \\ & & & e & u \\ l & l & & & r \end{bmatrix}, \text{where } s = 19.0,\ u = 21.0,\ p = 16.0,\ e = 5.0,\ r = 18.0,\ l = 12.0$$

SuperLU_DIST_2.0/FORTRAN/f_5x5.f90

```
 program f_5x5
use superlu_mod
 include 'mpif.h'
 implicit none
integer maxn, maxnz, maxnrhs
 parameter ( maxn = 10, maxnz = 100, maxnrhs
= 10 )
 integer colind(maxnz), rowptr(maxn+1)
 real*8  nzval(maxnz), b(maxn), berr(maxnrhs)
 integer n, m, nnz, nrhs, ldb, i, ierr, info, iam
 integer nprow, npcol
 integer init
 integer nnz_loc, m_loc, fst_row
 real*8  s, u, p, e, r, l

 integer(superlu_ptr) :: grid
integer(superlu_ptr) :: options
integer(superlu_ptr) :: ScalePermstruct
 integer(superlu_ptr) :: LUstruct
 integer(superlu_ptr) :: SOLVEstruct
 integer(superlu_ptr) :: A
 integer(superlu_ptr) :: stat
```

```
! Initialize MPI environment
      call mpi_init(ierr)

! Create Fortran handles for the C structures used
! in SuperLU_DIST
call f_create_gridinfo(grid)
call f_create_options(options)
call f_create_ScalePermstruct(ScalePermstruct )
call f_create_LUstruct(LUstruct)
call f_create_SOLVEstruct(SOLVEstruct)
call f_create_SuperMatrix(A)
call f_create_SuperLUStat(stat)

! Initialize the SuperLU_DIST process grid
    nprow = 1
    npcol = 2
    call f_superlu_gridinit
          (MPI_COMM_WORLD,
           nprow, npcol, grid)
    call get_GridInfo(grid, iam=iam)
```

f_5x5.f90 (cont.)

```
! Set up the input matrix A
! It is set up to use 2 processors:
!    processor 1 contains the first 2 rows
!    processor 2 contains the last 3 rows
        m    = 5
        n    = 5
        nnz = 12
        s    = 19.0
        u    = 21.0
        p    = 16.0
        e    = 5.0
        r    = 18.0
        l    = 12.0
if ( iam == 0 ) then
        nnz_loc    = 5
        m_loc      = 2
        fst_row    = 0        ! 0-based indexing
        nzval  (1) = s
        colind (1) = 0        ! 0-based indexing
        nzval  (2) = u
        colind (2) = 2
        nzval  (3) = u
        colind (3) = 3
        nzval  (4) = l
        colind (4) = 0
        nzval  (5) = u
        colind (5) = 1
        rowptr (1) = 0        ! 0-based indexing
        rowptr (2) = 3
        rowptr (3) = 5
else
        nnz_loc    = 7
        m_loc      = 3
        fst_row    = 2        ! 0-based indexing
        nzval  (1) = l
        colind (1) = 1
        nzval  (2) = p
        colind (2) = 2
        nzval  (3) = e
        colind (3) = 3
        nzval  (4) = u
        colind (4) = 4
        nzval  (5) = l
        colind (5) = 0
        nzval  (6) = l
        colind (6) = 1
        nzval  (7) = r
        colind (7) = 4
        rowptr (1) = 0        ! 0-based indexing
        rowptr (2) = 2
        rowptr (3) = 4
        rowptr (4) = 7
endif
```

f_5x5.f90 (cont.)

```
! Create the distributed compressed row matrix
! pointed to by the F90 handle
call f_dCreate_CompRowLoc_Matrix_dist
        (A, m, n, nnz_loc, m_loc, fst_row,     &
         nzval, colind, rowptr, SLU_NR_loc, &
         SLU_D, SLU_GE)
! Setup the right hand side
nrhs = 1
call  get_CompRowLoc_Matrix
           (A, nrow_loc=ldb)
do i = 1, ldb
    b(i) = 1.0
enddo

! Set the default input options
call f_set_default_options(options)

! Modify one or more options
Call set_superlu_options
       (options,ColPerm=NATURAL)
call  set_superlu_options
       (options,RowPerm=NOROWPERM)

! Initialize ScalePermstruct and LUstruct
call get_SuperMatrix (A,nrow=m,ncol=n)
call f_ScalePermstructInit(m, n, ScalePermstruct)
call f_LUstructInit(m, n, LUstruct)

! Initialize the statistics variables
call f_PStatInit(stat)

! Call the linear equation solver
call f_pdgssvx(options, A, ScalePermstruct, b,
        ldb, nrhs, grid, LUstruct, SOLVEstruct,
        berr, stat, info)

! Deallocate the storage allocated by SuperLU_DIST
call f_PStatFree(stat)
call f_Destroy_SuperMatrix_Store_dist(A)
call f_ScalePermstructFree(ScalePermstruct)
call f_Destroy_LU(n, grid, LUstruct)
call f_LUstructFree(LUstruct)
```

f_5x5.f90 (cont.)

```
! Release the SuperLU process grid
call f_superlu_gridexit(grid)

! Deallocate the C structures pointed to by the
! Fortran handles
call f_destroy_gridinfo(grid)
call f_destroy_options(options)
call f_destroy_ScalePermstruct(ScalePermstruct)
call f_destroy_LUstruct(LUstruct)
call f_destroy_SOLVEstruct(SOLVEstruct)
call f_destroy_SuperMatrix(A)
call f_destroy_SuperLUStat(stat)


! Terminate the MPI execution environment
call mpi_finalize(ierr)

Stop
end
```

Other Examples in EXAMPLE/

- Pddrive1.c:

  Solve the systems with same A but different right-hand side.
  - Reuse the factored form of A
- Pddrive2.c:

  Solve the systems with the same sparsity pattern of A.
  - Reuse the sparsity ordering
- Pddrive3.c:

  Solve the systems with the same sparsity pattern and similar values
  - Reuse the sparsity ordering and symbolic factorization
- Pddrive4.c:

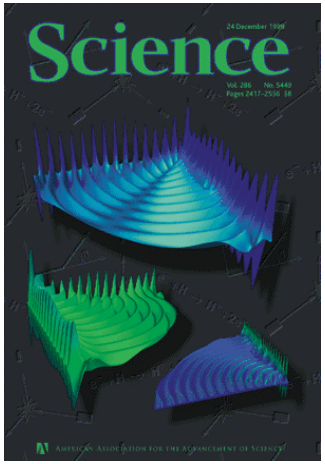
  Divide the processes into two subgroups (two grids) such that each subgroup solves a linear system independently from the other.

Application 1: Quantum Mechanics

- Scattering in a quantum system of three charged particles
- Simplest example is ionization of a hydrogen atom by collision with an electron:

$$e^- + H \rightarrow H^+ + 2e^-$$

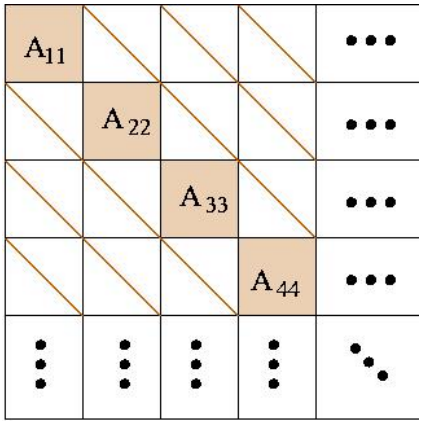
- Seek the particles' wave functions represented by the time-independent Schrodinger equation
- First solution to this long-standing unsolved problem [Recigno, McCurdy, et al. Science, 24 Dec 1999]



Quantum Mechanics (cont.)

- Finite difference leads to complex, unsymmetric systems, very ill-conditioned
  - Diagonal blocks have the structure of 2D finite difference Laplacian matrices

    Very sparse: nonzeros per row <= 13
  - Off-diagonal block is a diagonal matrix
  - Between 6 to 24 blocks, each of order between 200K and 350K
  - Total dimension up to 8.4 M



- Too much fill if use direct method . . .

SuperLU_DIST as Preconditioner

- SuperLU_DIST as block-diagonal preconditioner for CGS iteration

  $M^{-1}A\ x = M^{-1}b$

  $M = \mathrm{diag}(A_{11}, A_{22}, A_{33}, \ldots)$

- Run multiple SuperLU_DIST simultaneously for diagonal blocks
- No pivoting, nor iterative refinement

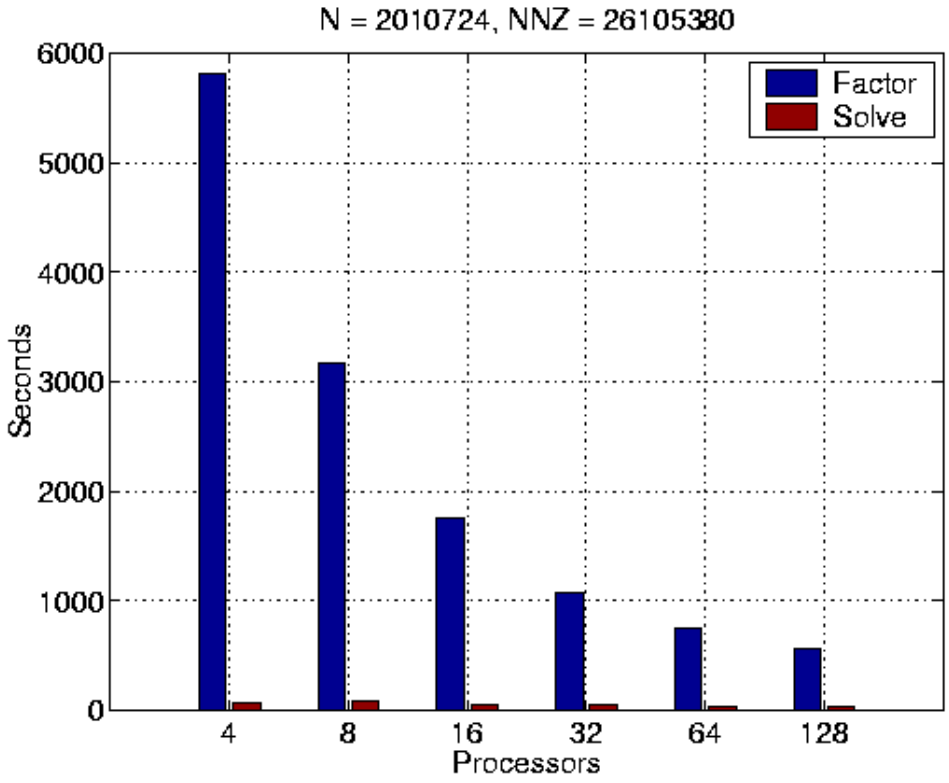
- 12 to 35 CGS iterations @ 1 ~ 2 minute/iteration using 64 IBM SP processors

  →Total time: 0.5 to a few hours

One Block Timings on IBM SP

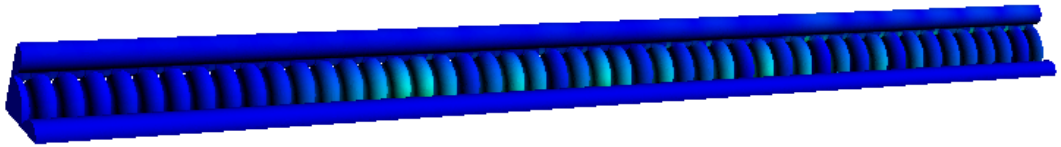
- Complex, unsymmetric

- N = 2 M, NNZ = 26 M
- Fill-ins using Metis: 1.3 G (50x fill)
- Factorization speed
  - 10x speedup (4 to 128 P)
  - Up to 30 Gflops



Application 2: Accelerator Cavity Design

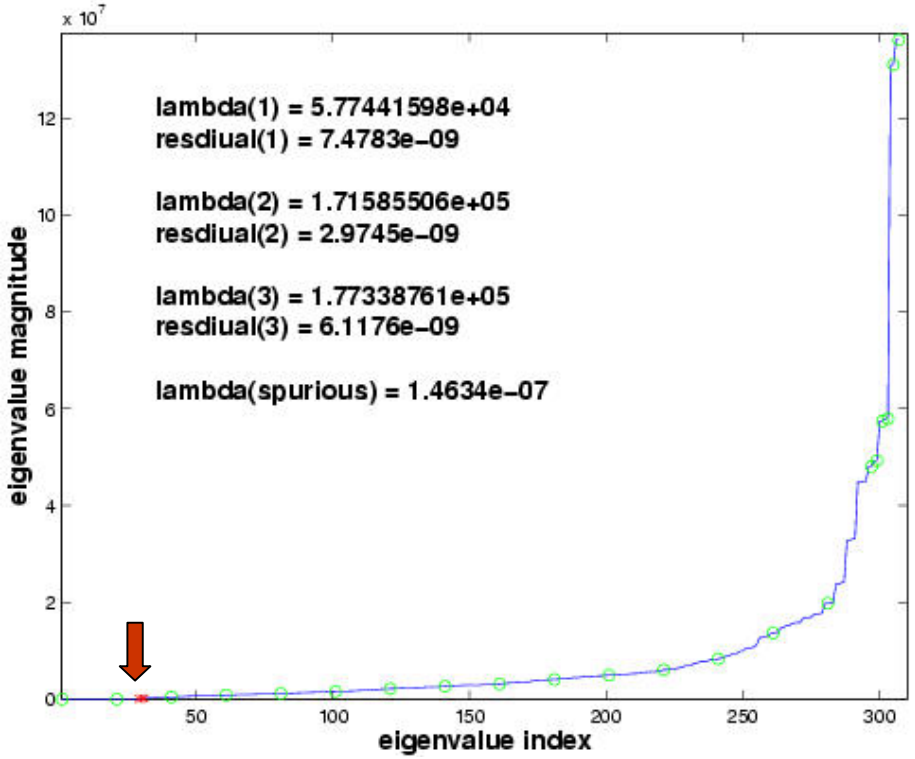
- Calculate cavity mode frequencies and field vectors
- Solve Maxwell equation in electromagnetic field
- Omega3P simulation code developed at SLAC



Omega3P model of a 47-cell section of the 206-cell Next Linear Collider accelerator structure

Individual cells used in accelerating structure

- Finite element methods lead to large sparse generalized eigensystem $\mathbf{K x} = \lambda \mathbf{M x}$
- Real symmetric for lossless cavities; Complex symmetric when lossy in cavities
- Seek interior eigenvalues (tightly clustered) that are relatively small in magnitude



Accelerator (cont.)

- Speed up Lanczos convergence by shift-invert

  ➔ Seek largest eigenvalues, well separated, of the transformed system

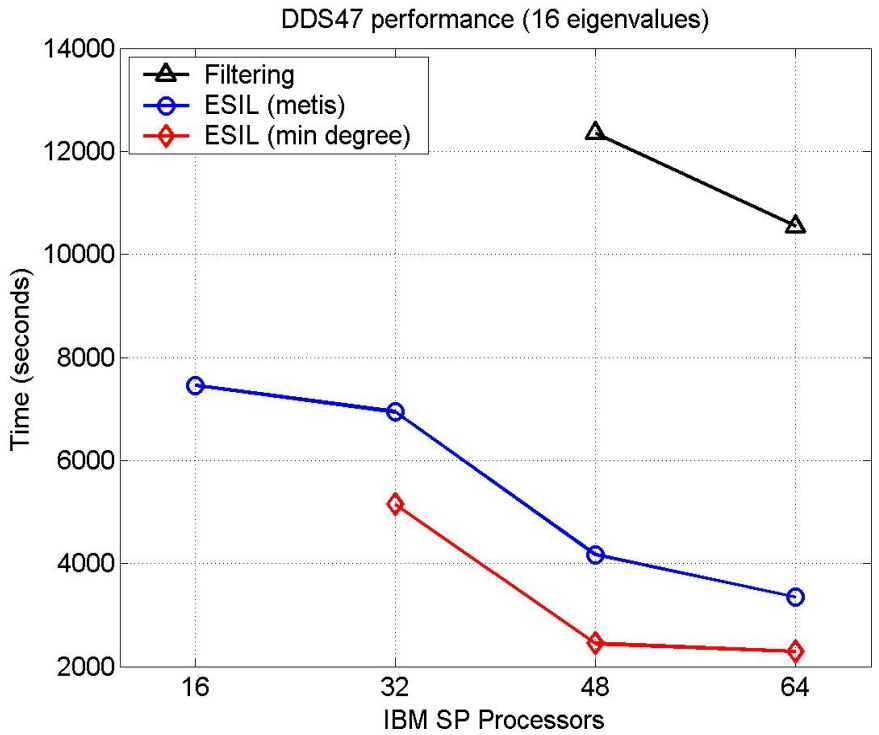
  $$M (K - \sigma M)^{-1} x = \mu M x$$

  $$\mu = 1 / (\lambda - \sigma)$$

- The Filtering algorithm [Y. Sun]
  - Inexact shift-invert Lanczos + JOCC (Jacobi Orthogonal Component Correction)
- We added exact shift-invert Lanczos (ESIL)
  - PARPACK for Lanczos
  - SuperLU_DIST for shifted linear system
  - No pivoting, nor iterative refinement

DDS47, Linear Elements

- Total eigensolver time: N = 1.3 M, NNZ = 20 M



Largest Eigen Problem Solved So Far

- DDS47, quadratic elements
  - N = 7.5 M, NNZ = 304 M
  - 6 G fill-ins using Metis

- 24 processors (8x3)
  - Factor: 3,347 s
  - 1 Solve: 61 s
  - Eigensolver: 9,259 s (~2.5 hrs)
    - 10 eigenvalues, 1 shift, 55 solves

Summary

- Efficient implementations of sparse LU on high-performance machines
- More sensitive to latency than dense case
- Continuing developments funded by TOPS and NPACI programs
  - Integrate into more applications
  - Improve triangular solution
  - Parallel ordering and symbolic factorization

- Survey of other sparse direct solvers: "Eigentemplates" book (www.netlib.org/etemplates)
  - LL^T, LDL^T, LU